

Supporting Information for

Decoupling factors influencing spatial and temporal trends of total nitrogen and ammonia nitrogen levels in lakes across China

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Supplementary table

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Introduction

This supplementary material provides additional information through supplementary table (Table S1-S2) to complement and support the conclusions in the main text.

Table S1 Hyperparameter configurations and optimization settings for the MLP-XGBoost stacking ensemble framework.

Model Component	Hyperparameter	Optimized Value / Setting
General Settings	Target Transformation	Log-transformation ($\ln(x+1)$)
	Feature Scaling	Z-score
	Temporal Encoding	Cyclic Sine/Cosine Transformation
Level-1: MLP	Hidden Layer Configuration	Branch: ($2 \times d_{in}$, $1 \times d_{in}$); Fusion: (64, 32)
	Activation Function	Rectified Linear Unit (ReLU)
	Attention Mechanism	Sigmoid-weighted Gating
	Optimizer	Adam ($LR=1 \times 10^{-3}$)
	Training Constraint	Early Stopping (Patience=15)
Level-1: XGBoost	Iterations($n_{estimators}$)	5,000 (with Early Stopping)
	Learning Rate	0.05
	Max Tree Depth	7
	Loss Function	Mean Squared Error (MSE)
	Regularization	$\lambda=0$, $\alpha=0$, $\gamma=0$
Level-2: Meta-Learner	Model Type	Ridge Regression
	Regularization	[0.1, 1.0, 10.0]

Table S2 Statistical significance of seasonal and regional variations in factor contributions based on Kruskal-Wallis tests.

Statistical category	Target Variable	Feature category	H statistic	p-value
Seasonal Variation	TN	External N Loading	149.61	< 0.001
		Hydro-climatic Dynamics	853.05	< 0.001
		Soil N Storage & Land Cover	3473.4	< 0.001
		Topography & Watershed Structure	2977.57	< 0.001
	NH	External N Loading	28989.73	< 0.001
		Hydro-climatic Dynamics	4032.34	< 0.001
		Soil N Storage & Land Cover	2551.51	< 0.001
		Topography & Watershed Structure	36740.81	< 0.001
limnological zones Variation	TN	External N Loading	1380.8	< 0.001
		Hydro-climatic Dynamics	825.87	< 0.001
		Soil N Storage & Land Cover	5207.59	< 0.001
		Topography & Watershed Structure	4245.7	< 0.001
	NH	External N Loading	20948.41	< 0.001
		Hydro-climatic Dynamics	4688.88	< 0.001
		Soil N Storage & Land Cover	2756	< 0.001
		Topography & Watershed Structure	28032.63	< 0.001